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A comparison of algorithms for the multivariate L_1-median

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Abstract The L_1-median is a robust estimator of multivariate location with good statistical properties. Several algorithms for computing the L_1-median are available. Problem specific algorithms can be used, but also general optimization routines. The aim is to compare different algorithms with respect to their precision and runtime. This is possible because all considered algorithms have been implemented in a standardized manner in the open source environment R. In most situations, the algorithm based on the optimization routine NLM (non-linear minimization) clearly outperforms other approaches. Its low computation time makes applications for large and high-dimensional data feasible.

Keywords Algorithm · Multivariate median · Optimization · Robustness

1 Introduction

A prominent generalization of the univariate median to higher dimensions is the geometric median, also called L_1-median. For a data set $\boldsymbol{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ with each

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$\boldsymbol{x}_i \in I\!R^p$, the L_1-median $\hat{\boldsymbol{\mu}}$ is defined as

$$\hat{\boldsymbol{\mu}}(\boldsymbol{X}) = \underset{\boldsymbol{\mu}}{\operatorname{argmin}} \sum_{i=1}^{n} \|\boldsymbol{x}_i - \boldsymbol{\mu}\| \tag{1}$$

where $\|\cdot\|$ denotes the Euclidean norm. In words, the L_1-median is the point for which the sum of the Euclidean distances to n given data points is minimal. This problem is formulated in an even more general form by Weber (1909) (*Fermat-Weber problem*), as he refers to location issues in industrial contexts. If the data points are not collinear, the solution to problem (1) is unique (Weiszfeld, 1937). The L_1-median has several further attractive statistical properties, like:

(a) Its breakdown point is 0.5 (Lopuhaä and Rousseeuw, 1991), i.e., only if more than 50% of the data points are contaminated, the L_1-median can take values beyond all bounds.

(b) It is location and orthogonally equivariant, that is for any $\boldsymbol{b} \in I\!R^p$ and orthogonal $p \times p$ matrix $\boldsymbol{L}$,
$$\hat{\boldsymbol{\mu}}(\boldsymbol{L}\boldsymbol{X} + \boldsymbol{b}) = \boldsymbol{L}\hat{\boldsymbol{\mu}}(\boldsymbol{X}) + \boldsymbol{b},$$
with $\boldsymbol{L}\boldsymbol{X} + \boldsymbol{b} = \{\boldsymbol{L}\boldsymbol{x}_1 + \boldsymbol{b}, \ldots, \boldsymbol{L}\boldsymbol{x}_n + \boldsymbol{b}\}$.

Property (a) makes this estimator very attractive from a robustness point of view. According to property (b), the L_1-median is orthogonal equivariant, but not affine equivariant. Orthogonal equivariance is already sufficient for many situations, like for principal component analysis (PCA). Therefore several authors consider the L_1-median in the context of robust PCA (e.g., Croux and Ruiz-Gazen, 2005; Croux et al, 2007).

An iterative algorithm for finding the numerical solution of the L_1-median has been proposed by Weiszfeld (1937). Several other algorithms will be outlined in Section 2. The goal of this paper is to compare the algorithms with respect to their precision and runtime (Section 3). For such a comparison, a unified implementation of the algorithms has been made using C++ code embedded in the R-library `pcaPP` (R Development Core Team, 2010), see Section 2.3. The final Section 4 concludes.

2 Algorithms for computing the L_1-median

For the computation of the estimate $\hat{\boldsymbol{\mu}}$ we have to minimize the convex function

$$S(\boldsymbol{\mu}) = \sum_{i=1}^{n} \|\boldsymbol{x}_i - \boldsymbol{\mu}\|. \tag{2}$$

The algorithms tested and examined here can generally be divided into two categories:

2.1 General optimization procedures

The minimization of (2) can be done by numerical algorithms, developed for general, non-linear optimization purposes. One can either evaluate the target function $S(\boldsymbol{\mu})$ on several points, or additionally use the first derivative of $S(\boldsymbol{\mu})$,

$$\frac{\partial S(\boldsymbol{\mu})}{\partial \boldsymbol{\mu}} = -\sum_{i=1}^{n} \frac{\boldsymbol{x}_i - \boldsymbol{\mu}}{\|\boldsymbol{x}_i - \boldsymbol{\mu}\|}, \tag{3}$$

or the Hessian matrix

$$\frac{\partial^2 S(\boldsymbol{\mu})}{\partial \boldsymbol{\mu}\, \partial \boldsymbol{\mu}^t} = \sum_{i=1}^{n} \left(\frac{1}{\|\boldsymbol{x}_i - \boldsymbol{\mu}\|}\, \boldsymbol{I}_p - \frac{(\boldsymbol{x}_i - \boldsymbol{\mu})(\boldsymbol{x}_i - \boldsymbol{\mu})^t}{\|\boldsymbol{x}_i - \boldsymbol{\mu}\|^3} \right), \tag{4}$$

where $\boldsymbol{I}_p$ is the $p \times p$ identity matrix . Since all algorithms are implemented in the software environment R (R Development Core Team, 2010), we considered general unconstrained non-linear optimization algorithms which are accessible in this environment for our purpose:

- **NM:** Nelder and Mead (1965) proposed a simplex method for minimizing functions of p variables, also known as downhill simplex method. Values of the target function are compared at $p+1$ points, whereas the point with highest target value is replaced in each iteration. Rather many iterations are needed till convergence, but as this is one of the most common simplex algorithms, it is included in this comparison.
- **BFGS:** Broyden, Fletcher, Goldfarb and Shanno proposed a quasi-Newton algorithm searching for a stationary point of a function by local quadratic approximation (see, e.g., Nocedal and Wright, 2006). In contrast to *real* Newton methods, this algorithm does not require an analytical computation of the exact Hessian matrix, as this is approximated internally by the algorithm. Since in high-dimensional situations the computation of the exact Hessian matrix can be quite time consuming, algorithms that approximate the Hessian matrix internally are to be preferred in this context.
- **CG:** Conjugate gradient algorithms are iterative methods, known for their low memory requirements. Quasi-Newton methods usually converge after fewer iterations, but a single iteration of a conjugate gradient method is computationally less intensive. In the subsequent simulations, the version of Fletcher and Reeves (1964) is applied. The gradient information in equation (3) is used by this method.
- **NLM:** Non-linear minimization can be carried out by a Newton-type algorithm (Dennis and Schnabel, 1983), using the gradient information from equation (3). It provides two options regarding the Hessian matrix: an analytical representation can be provided, or the Hessian matrix is again approximated internally by secant methods. Approximating the Hessian matrix turned out to be the faster approach, particularly when high-dimensional data sets are processed. Hence in subsequent simulations the Hessian matrix is always approximated rather than analytically calculated. From the three available optimization types introduced in Dennis and Schnabel (1983), *Line Search*, *Double Dogleg*, and *More-Hebdon*, the first method is applied here, as in this context its convergence characteristics turned out to be most reliable among these three.

2.2 Problem specific algorithms

For the specific problem of computing the L_1-median, several algorithms have been proposed in the literature. Here we mention the algorithm of Weiszfeld (1937), which is the basis for an improved version by Vardi and Zhang (2000). Another algorithm, based on the steepest descent, has been introduced by Hössjer and Croux (1995), and will also be examined here.

- Weiszfeld (1937) formulated an iterative approach for solving the Fermat-Weber problem for data points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ and n non-negative weights. In this paper all

weights are equal. A current (or initial) solution $\hat{\boldsymbol{\mu}}_l$ is improved by calculating a scaled sum of all observations:

$$T_0(\boldsymbol{\mu}) = \frac{\sum_{i=1}^{n} \frac{\boldsymbol{x}_i}{\|\boldsymbol{x}_i - \boldsymbol{\mu}\|}}{\sum_{i=1}^{n} \frac{1}{\|\boldsymbol{x}_i - \boldsymbol{\mu}\|}} \tag{5}$$

$$\hat{\boldsymbol{\mu}}_{l+1} = \begin{cases} T_0(\hat{\boldsymbol{\mu}}_l) & \text{if } \hat{\boldsymbol{\mu}}_l \notin \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\} \\ \hat{\boldsymbol{\mu}}_l & \text{if } \hat{\boldsymbol{\mu}}_l \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\} \end{cases} \tag{6}$$

This algorithm converges given that $\hat{\boldsymbol{\mu}}_l \notin \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ for every iteration step $l \in \mathbb{N}$.

- **VaZh:** Vardi and Zhang (2000) improved the behavior of Weiszfeld's algorithm in case that $\hat{\boldsymbol{\mu}}_l \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ appears in any iteration. The resulting algorithm is, apart from the treatment of this particular issue, quite similar, and for this reason no comparison is made with Weiszfeld's original algorithm later on in the simulation study. The proposal of Vardi and Zhang (2000) is as follows:

$$T_1(\boldsymbol{\mu}) = \frac{\sum_{\boldsymbol{x}_i \neq \boldsymbol{\mu}} \frac{\boldsymbol{x}_i}{\|\boldsymbol{x}_i - \boldsymbol{\mu}\|}}{\sum_{\boldsymbol{x}_i \neq \boldsymbol{\mu}} \frac{1}{\|\boldsymbol{x}_i - \boldsymbol{\mu}\|}} \tag{7}$$

$$\eta(\boldsymbol{\mu}) = \begin{cases} 1 & \text{if } \boldsymbol{\mu} = \boldsymbol{x}_i,\ i = 1, \ldots, n \\ 0 & \text{else} \end{cases} \tag{8}$$

$$R(\boldsymbol{\mu}) = \sum_{\boldsymbol{x}_i \neq \boldsymbol{\mu}} \frac{\boldsymbol{x}_i - \boldsymbol{\mu}}{\|\boldsymbol{x}_i - \boldsymbol{\mu}\|} \tag{9}$$

$$\gamma(\boldsymbol{\mu}) = \min\left(1, \frac{\eta(\boldsymbol{\mu})}{\|R(\boldsymbol{\mu})\|}\right) \tag{10}$$

$$\hat{\boldsymbol{\mu}}_{l+1} = (1 - \gamma(\hat{\boldsymbol{\mu}}_l))\, T_1(\hat{\boldsymbol{\mu}}_l) + \gamma(\hat{\boldsymbol{\mu}}_l)\hat{\boldsymbol{\mu}}_l. \tag{11}$$

The case $\hat{\boldsymbol{\mu}}_l \notin \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ implies $\gamma(\hat{\boldsymbol{\mu}}_l) = 0$, and the algorithm behaves exactly as in (5). Otherwise, if $\hat{\boldsymbol{\mu}}_l \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$, the sum in (7) is calculated as in (5), but only over the $\boldsymbol{x}_i \neq \hat{\boldsymbol{\mu}}_l$, whereas observation $\boldsymbol{x}_i = \hat{\boldsymbol{\mu}}_l$ is added afterwards in (11), applying weight $\gamma(\hat{\boldsymbol{\mu}}_l)$.

- **HoCr:** Hössjer and Croux (1995) proposed an approach which combines a steepest descent algorithm with step halving. The current solution is improved by stepping into the direction with steepest descent of the target function. If the target function increases after this step, the step size is being halved until the target function decreases. If the step size shrinks to zero without finding a better solution, the algorithm has converged. A detailed description of the algorithm including pseudocode is given by the authors. Their algorithm can also be used for the rank based extension of the L_1-median they propose.

For reasons of completeness, let us mention two other algorithms proposed in the literature for computing the L_1-median. Gower (1974) proposed a steepest descent algorithm combined with a bisection algorithm. It is somehow similar to the HoCr algorithm, but the use of the bisection method instead of step-halving considerably increases the computation time. Bedall and Zimmermann (1979) proposed to use the Newton-Raphson procedure with the exact expression (4) for the Hessian matrix, and

is similar to the NLM method with analytical second derivative. It turned out to be much slower than the NLM procedure. The algorithms of Gower (1974) and Bedall and Zimmermann (1979) are included in the R-package `depth`. Due to their similarity with algorithms already included in the simulation study, and since they are not competitive in terms of computation speed, we do not report their performance in this paper.

2.3 Implementation

Due to efficiency issues (runtime and memory), all methods are implemented in C++ and are embedded in the R-library `pcaPP` (version 1.8-1). The algorithms based on general optimization methods are simply wrapping the available routines in R, see Table 1. The routine for non-linear minimization (`optif9`) originates from the UNCMIN-

Algorithm	R - Optimizer	`pcaPP` - Routine
Nelder and Mead (NM)	`nmmin`	`l1median_NM`
Broyden, Fletcher, Goldfarb and Shanno (BFGS)	`vmmin`	`l1median_BFGS`
Conjugate gradient (CG)	`cgmin`	`l1median_CG`
Non-linear minimization (NLM)	`optif9`	`l1median_NLM`
Vardi and Zhang (VaZh)		`l1median_VaZh`
Hössjer and Croux (HoCr)		`l1median_HoCr`

Table 1 Implementation of the optimization methods as wrapper functions.

Fortran package by R.B. Schnabel which implements Newton and quasi-Newton algorithms for unconstrained minimization, see Dennis and Schnabel (1983), Schnabel et al (1985). All other mentioned routines are C-implementations which come along with R. By default the component-wise median is used as starting value for all mentioned algorithms.

The more specific L_1-median routines (Vardi and Zhang, 2000; Hössjer and Croux, 1995) are transcripts of the routines published in the R-library `robustX`, whereas the original implementation of the algorithm by Hössjer and Croux (1995) was made available by the authors. The implementation of the algorithm of Vardi and Zhang (2000) is changed slightly, as the original algorithm crashes if $\boldsymbol{\mu} = \boldsymbol{x}_i$ for more than one $i \in \{1, \ldots, n\}$, see equation (8). Although this might be a rare situation, equation (8) needs to be changed to

$$\eta(\boldsymbol{\mu}) = \sum_{\boldsymbol{x}_i = \boldsymbol{\mu}} 1 \tag{12}$$

in order to stabilize the algorithm in such degenerated cases.

2.4 Convergence

When comparing different ways of solving a problem, one major issue is to create equal and thus fair conditions for each approach which is to be examined. Here each algorithm can be tested providing exactly the same input, whereas the output quality can be compared likewise by checking the value of the target function $S(\hat{\boldsymbol{\mu}})$ of (2). However,

it is not as easy to control the precision of the results of each particular algorithm. Each of the mentioned algorithms provides an input control parameter τ, which is a tolerance level influencing the convergence behavior, and is mainly used to specify the desired precision. Unfortunately this tolerance level is interpreted differently, as shown in Table 2.

Algorithm	Convergence criterion	Based on
NM BFGS CG	$S\left(\hat{\boldsymbol{\mu}}_{l-1}\right) - S\left(\hat{\boldsymbol{\mu}}_l\right) \leq \tau\left(S\left(\hat{\boldsymbol{\mu}}_l\right) + \tau\right)$	Relative change of $S\left(\hat{\boldsymbol{\mu}}\right)$
NLM	$\nabla := \frac{\left\lvert \frac{\partial S(\hat{\boldsymbol{\mu}}_l)}{\partial \hat{\boldsymbol{\mu}}_l} \right\rvert \max\{\lVert\hat{\boldsymbol{\mu}}_l\rVert, 1\}}{\max\{\lvert S(\hat{\boldsymbol{\mu}}_l)\rvert, 1\}}$ $\max_i \nabla_i \leq \tau$ with $\nabla = (\nabla_1, \ldots, \nabla_p)^t$	Maximum scaled gradient
VaZh	$\lVert\hat{\boldsymbol{\mu}}_{l-1} - \hat{\boldsymbol{\mu}}_l\rVert_1 \leq \tau\lVert\hat{\boldsymbol{\mu}}_l\rVert_1$	Relative change of $\hat{\boldsymbol{\mu}}$ (L_1-norm)
HoCr	$\lVert\hat{\boldsymbol{\mu}}_{l-1} - \hat{\boldsymbol{\mu}}_l\rVert_2 \leq \tau$	Change of $\hat{\boldsymbol{\mu}}$ (L_2-norm)

Table 2 Convergence criteria for different optimization routines.

In order to still get comparable results, we have to choose τ appropriately. This is done by examining first, which tolerance level τ leads to comparable precision in a particular situation, and then these tolerance levels are applied in all subsequent simulation settings. Details are provided in the next section.

3 Comparison of the algorithms

In order to test the performance of the algorithms, several types of artificial and real data samples are chosen. On a particular data set, the L_1-median is computed with each algorithm discussed above and the resulting estimations are compared by considering the values of the target function (2). The smallest resulting target value is used as reference, whereas deviations from this reference value indicate worse approximations of the L_1-median. Throughout this paper this relative quality measure is referred to as the *deviation*. The best algorithm(s) always yield a deviation of exactly zero. In the following simulated scenarios, each simulation is performed 100 times with data sets sampled from the same distribution. As measure for overall precision the 95% quantile of the resulting deviations is considered, referred to as the *95% deviation quantile*. The motivation for this measure is that it reflects the precision of the vast majority of runs, but does not account for single runs where the convergence behavior was different just by chance. Additionally, the (median) runtime in seconds is reported for each algorithm. All simulations are computed on an AMD Athlon 64 X2 4200+ Processor at 2.2 GHz.

In order to stop non converging algorithms from freezing the process, the maximum number of iterations is set to 500 for each algorithm. If not stated differently, the simulated data sets consist of $n = 1000$ observations and $p = 100$ variables. The covariance matrix $\boldsymbol{C}$ of the distribution used to generate the data is diagonal with diagonal elements $p + 1 - i$, for $i = 1, \ldots, p$. Outliers are generated by randomly

selecting observations from the simulated data matrix, multiplying them with a value of 10, and shifting them in each coordinate by the value 10.

3.1 Adjusting tolerance levels for convergence

Before comparing any results of the different algorithms, their convergence criteria shall be examined and their tolerance levels need to be adjusted, such that they deliver equal precision for a particular simulation setting. For that purpose a simple simulation is performed with several tolerance levels τ, monitoring the resulting precisions. This allows to obtain a tolerance level for each algorithm leading to similar precisions. In the subsequent simulations, these tolerance levels are used and so the resulting figures are directly comparable. The algorithms are applied to 100 different p-variate normally distributed data sets (we used $n = 1000$ and $p = 100$ in the following) with center $\mathbf{0}$, covariance matrix $\boldsymbol{C}$ (see above) and without outliers. The tolerance level is altered between 1e-1 and 1e-20. Figure 1 shows the 95% deviation quantiles of each algorithm computed over different tolerance levels. Note that a 95% deviation quantile of exactly 0 has been truncated to 1e-15 for being able to use logarithmic scales. A value of 1e-15 (or below) is reached at a tolerance level of 1e-5 for HoCr, at 1e-6 for VaZh, at 1e-9 for CG, and at 1e-11 for NLM. This high precision cannot be reached for the algorithms BFGS and NM within the considered range of the tolerance levels; NM seems to be totally unaffected by the choice of the tolerance level. Also changing the different tuning parameters of the algorithm NM does not lead to better results in a simulation as presented here.

Considering the computation time of the algorithms with respect to the used tolerance level (Figure 2), it is noticeable that the algorithm NLM seems to be rather unaffected by the desired output precision. CG shows a large increase in runtime when τ is raised from 1e-11 to 1e-13.

Table 3 shows the chosen tolerance levels for subsequent simulations. The largest level of τ at which each algorithm reaches its best performance (zero deviation) is chosen and then scaled down by a factor 1e3, compensating for different simulation scenarios, as the data structure might slightly influence the convergence behavior. With respect to the high increase of the runtime of the algorithm CG when τ excesses 1e-11, this algorithm's tolerance level is set to 1e-10. As method NM does not seem to be affected by the tolerance level, the choice of τ = 1e-10 is admittedly arbitrary.

NM	BFGS	CG	NLM	VaZh	HoCr
1e-10	1e-17	1e-10	1e-14	1e-9	1e-8

Table 3 Tolerance levels τ as used for each particular algorithm.

3.2 Uncorrelated data

The observations are drawn randomly from p-variate normal (N_p) and log-normal (LN_p) distributions, respectively, with center $\mathbf{0}$ and covariance matrix $\boldsymbol{C}$. Simulations

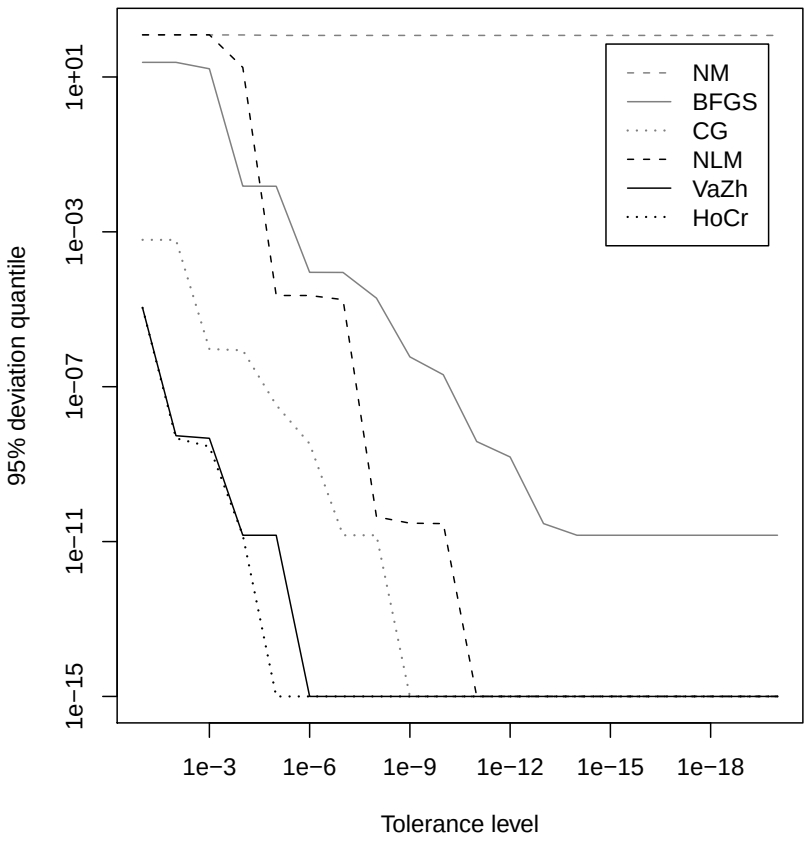

Fig. 1 The 95% deviation quantiles of the L_1-median target values as a function of the tolerance level τ.

on multivariate t-distributed data have been computed too, but as the algorithms perform quite similar as on normally distributed data, these results are omitted here. In order to get an impression on how the algorithms are relatively affected by outliers, the percentage of outliers, p_{out}, varies between 0% and 40% . Table 4 shows the 95% deviation quantiles of each algorithm, for the given distributions and different percentages of outliers. For $p_{out} = 0$ (and normally distributed data) this is the same simulation setting as before when the tolerance levels have been chosen, and it is not surprising that apart from BFGS and NM all algorithms return the same precision, yielding a 95% deviation quantile of 0. As the concept of the L_1-median may downweight but never completely trims any observation, added outliers always slightly influence the estimation. However, increasing p_{out} does not influence the algorithms' relative performance, as none of the methods can be identified as particularly sensitive to a different outlier proportion among the tested candidates. The runtime behavior in this simulation setting is shown in Table 5. It is not possible to point out one algorithm which is always the fastest while delivering the best approximation quality. On normally distributed data, BFGS is the fastest algorithm, but as seen before it is not as accurate as other

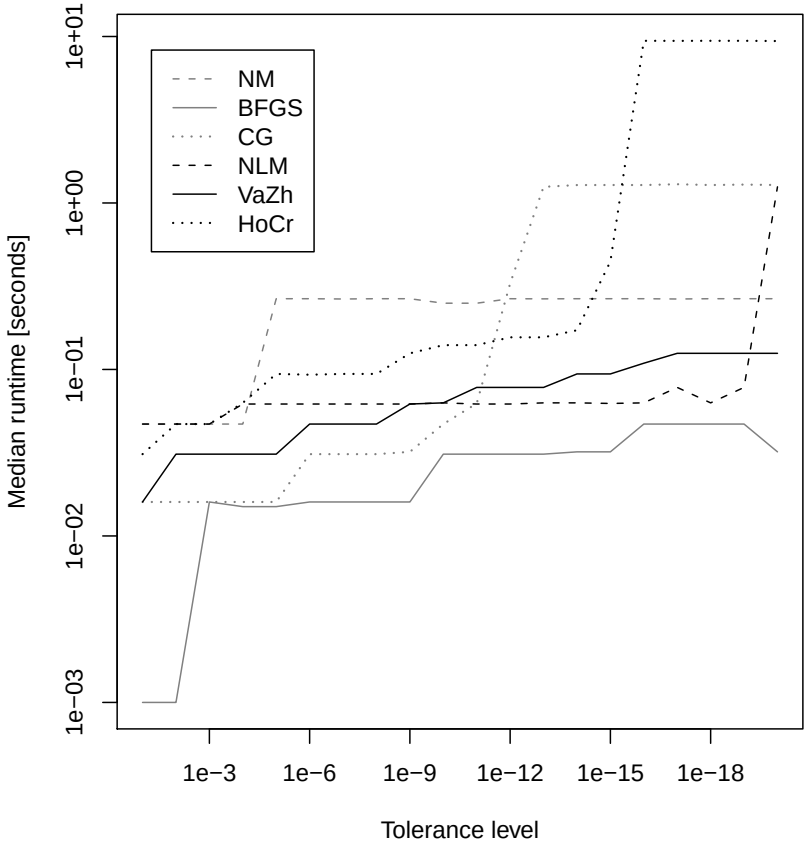

Fig. 2 Median runtimes [seconds] of the L_1-median computation as a function of the tolerance level τ.

methods. The runtimes of the algorithms seem to be quite independent from the added amount of outliers, and they are all in about the same range (apart from NM being always the slowest choice which obviously is caused by convergence issues). Applying the algorithms on log-normally distributed data, however, yields the best results for the NLM algorithm. In terms of computation time, NLM is the only algorithm which is not heavily influenced by the distribution type, nor by the amount of outliers added. For the algorithms VaZh, HoCr and CG, the data configuration has a notable effect since their runtimes increase up to a factor of 6 (CG) when highly contaminated data are processed. The algorithm of Nelder and Mead (NM) never converges within the 500 allowed iterations, which explains its high deviation values and longer runtimes.

3.3 Correlated data

In this section we investigate the effect of a correlation structure within the simulated data on the performance of the algorithms. Therefore, we use a covariance matrix $\boldsymbol{C'}$

Distribution	p_{out}	NM	BFGS	CG	NLM	VaZh	HoCr
$N_p(\mathbf{0}, \mathbf{C})$	0 %	115	1.46e-11	0	0	0	0
	10 %	118	2.91e-11	0	0	0	0
	20 %	133	1.46e-12	0	0	0	0
	30 %	147	0	0	0	0	0
	40 %	146	5.82e-11	0	0	0	0
$LN_p(\mathbf{0}, \mathbf{C})$	0 %	1.66	1.19e-13	0	0	0	0
	10 %	3.51	4.77e-13	0	0	0	0
	20 %	5.98	9.09e-13	0	0	0	0
	30 %	9.60	9.09e-13	0	0	0	0
	40 %	16.20	1.82e-12	0	0	0	0

Table 4 95% deviation quantiles of L_1-median algorithms applied to uncorrelated data.

Distribution	p_{out}	NM	BFGS	CG	NLM	VaZh	HoCr
$N_p(\mathbf{0}, \mathbf{C})$	0 %	0.265	0.032	0.047	0.063	0.062	0.094
	10 %	0.266	0.046	0.125	0.063	0.062	0.078
	20 %	0.265	0.032	0.047	0.063	0.062	0.078
	30 %	0.265	0.031	0.046	0.063	0.062	0.078
	40 %	0.265	0.031	0.047	0.063	0.062	0.078
$LN_p(\mathbf{0}, \mathbf{C})$	0 %	0.266	0.172	0.047	0.063	0.062	0.078
	10 %	0.266	0.172	0.281	0.063	0.062	0.078
	20 %	0.265	0.187	0.109	0.078	0.078	0.109
	30 %	0.265	0.141	0.211	0.078	0.110	0.141
	40 %	0.265	0.109	0.297	0.078	0.218	0.250

Table 5 Median runtimes [seconds] of the L_1-median algorithms applied to uncorrelated data.

for data generation, with elements 1 in the diagonal, and numbers c as off-diagonal elements. The values of c are set to 0.5, 0.9, and 0.99 among the different simulation scenarios. In addition, the effect of the data distribution and the influence of outliers is observed. Table 6 shows the precision of the algorithms. Their performance does not seem to be really influenced by the correlation level c, the only difference is observed for the algorithm HoCr which performs slightly worse for log-normally distributed highly correlated data.

According to Table 7, the only algorithms unaffected by the correlation level are NM and NLM. NM again did not converge which explains the constant runtime of 265 milliseconds. NLM however converges almost within the same time as when applied on uncorrelated data, which is outstanding among all tested methods. The algorithms CG, HoCr and VaZh require more computation time for highly correlated data.

3.4 High-dimensional data with low sample size ($p \gg n$)

Here we generate data according to $N_p(\mathbf{0}, \boldsymbol{I}_p)$ and $LN_p(\mathbf{0}, \boldsymbol{I}_p)$, respectively, for $n = 10$ and $p = 100$. As previously, contamination is added and its percentage is varied. Since the rank of the generated p-dimensional data is n, it is possible to reduce the dimensionality to n without any loss of information. This is done by singular value decomposition (SVD) as follows (compare Serneels et al, 2005). Let $\boldsymbol{X}$ be the simulated data matrix, then $\boldsymbol{X}^t = \boldsymbol{V}\boldsymbol{S}\boldsymbol{U}^t$ is the SVD of $\boldsymbol{X}^t$, with $\boldsymbol{U}$ an $n \times n$ orthogonal matrix, $\boldsymbol{S}$ a diagonal matrix including the n singular values in its diagonal, and $\boldsymbol{V}$ a

Distribution	p_{out}	r	NM	BFGS	CG	NLM	VaZh	HoCr
$N_p(\mathbf{0}, \mathbf{C}')$	0 %	0.5	19.2	1.82e-12	0	0	0	0
		0.9	23.3	1.82e-12	0	0	0	0
		0.99	31.0	1.82e-12	0	0	0	0
	30 %	0.5	33.2	7.28e-12	0	0	0	0
		0.9	22.1	7.28e-12	0	0	0	0
		0.99	57.8	7.28e-12	0	0	0	0
$LN_p(\mathbf{0}, \mathbf{C}')$	0 %	0.5	3.09	1.14e-13	0	0	0	0
		0.9	2.83	1.14e-13	0	0	0	1.14e-13
		0.99	4.34	1.14e-13	0	0	0	2.27e-13
	30 %	0.5	3.62	9.09e-13	0	0	0	0
		0.9	3.13	9.09e-13	0	0	0	0
		0.99	3.42	9.09e-13	0	0	0	9.09e-13

Table 6 95% deviation quantiles of L_1-median algorithms applied to correlated data.

Distribution	p_{out}	c	NM	BFGS	CG	NLM	VaZh	HoCr
$N_p(\mathbf{0}, \mathbf{C}')$	0 %	0.5	0.265	0.078	0.110	0.063	0.156	0.219
		0.9	0.265	0.094	0.296	0.078	0.281	0.422
		0.99	0.265	0.125	0.344	0.078	0.468	0.688
	30 %	0.5	0.265	0.063	0.297	0.078	0.156	0.188
		0.9	0.265	0.078	0.593	0.078	0.250	0.328
		0.99	0.265	0.110	0.718	0.078	0.422	0.547
$LN_p(\mathbf{0}, \mathbf{C}')$	0 %	0.5	0.266	0.157	0.141	0.078	0.156	0.203
		0.9	0.265	0.156	0.211	0.078	0.282	0.359
		0.99	0.266	0.140	0.375	0.078	0.453	0.570
	30 %	0.5	0.265	0.094	0.539	0.078	0.172	0.203
		0.9	0.265	0.156	0.609	0.078	0.265	0.313
		0.99	0.266	0.141	1.258	0.078	0.406	0.500

Table 7 Median runtimes [seconds] of the L_1-median algorithms applied to correlated data.

$p \times n$ orthogonal matrix. The matrix $\tilde{\boldsymbol{X}} = \boldsymbol{U}\boldsymbol{S}$ has only size $n \times n$, but it contains the same information as $\boldsymbol{X}$. Using this dimension reduction, we can apply the L_1-median algorithms to both $\boldsymbol{X}$ and $\tilde{\boldsymbol{X}}$, and compare the resulting estimates $\hat{\boldsymbol{\mu}}$ and $\hat{\tilde{\boldsymbol{\mu}}}$, respectively. This can be done by back-transforming the column vector $\hat{\tilde{\boldsymbol{\mu}}}$ to the original space with $\boldsymbol{V}\hat{\tilde{\boldsymbol{\mu}}}$, and comparing the results with the Euclidean distance

$$\delta = \|\hat{\boldsymbol{\mu}} - \boldsymbol{V}\hat{\tilde{\boldsymbol{\mu}}}\|. \tag{13}$$

This difference between estimations in transformed and original space is computed 100 times for each simulation setting, and the 95% distance quantile is reported in Table 8. As the algorithm NLM provided the best results in previous simulations, it is rather expected that it also performs well in here. Indeed, this is confirmed, as NLM gives the smallest distances between the estimations computed in the original and in the transformed space. The only algorithm which sticks out again due to its instability and inaccuracy is NM, which has to be stopped after 500 iterations without reaching convergence.

Distribution	p_{out}	NM	BFGS	CG	NLM	VaZh	HoCr
$N_p(\mathbf{0}, \boldsymbol{I}_p)$	0 %	3.98	2.71e-07	2.93e-07	7.31e-12	8.49e-10	9.41e-08
	10 %	3.81	2.37e-07	2.81e-07	7.41e-12	8.27e-10	1.13e-07
	20 %	4.42	2.32e-07	3.21e-07	1.14e-11	1.04e-09	1.21e-07
	30 %	4.92	3.54e-07	3.57e-07	1.53e-11	1.06e-09	1.66e-07
	40 %	5.71	4.6e-07	4.1e-07	1.77e-11	1.51e-09	2.07e-07
$LN_p(\mathbf{0}, \boldsymbol{I}_p)$	0 %	0.0401	2.46e-09	2.57e-09	6.44e-15	8.41e-12	3.74e-10
	10 %	0.0376	2.27e-09	2.58e-09	8.19e-15	8.07e-12	1.22e-09
	20 %	0.0424	3.29e-09	2.88e-09	1.47e-14	1.17e-11	1.99e-09
	30 %	0.0464	5.24e-09	3.69e-09	2.78e-14	1.79e-11	3.56e-09
	40 %	0.0591	6.06e-09	6.08e-09	4.97e-14	1.41e-10	7.46e-09

Table 8 95% distance quantiles of L_1-median algorithms applied to the original and the transformed data sets.

3.5 Degenerated situations

In this subsection we study the behavior of the algorithms at two particular data structures. First we consider the case of collinear data, secondly the case where more than half of the data points are coinciding. In these settings the exact value of the minimum of the objective function (2) is known. The deviation of an algorithm is now computed relative to the exact optimum.

- If n is even, and all observations are collinear, the L_1-median is not uniquely defined, as any point between the 2 innermost observations is a proper solution (this is in analogy to the univariate median). As such a data structure has rank one, the application of the classical median is possible yielding the same result as the L_1-median. Therefore the data matrix has to be projected onto the line given by two arbitrary (different) observations, which in this case coincidences with the first principal component. The median is computed in this one-dimensional subspace, whereas the result is transformed back into the original space afterwards.
  Simulations on data sets generated with a covariance matrix with arbitrary values (finite and positive) for the variances, and off-diagonal elements $c_{ij} = \sqrt{(c_{ii}c_{jj})}$ $\forall i \neq j$ (perfect collinearity of all variables) and arbitrary (finite) mean vectors result in Table 9. Apart from two occurrences where VaZh gives slightly better results, the algorithms CG, NLM, VaZh and HoCr show equal performance and return an exact solution. BFGS still returns good results but seems to have numerical problems due to its slight imprecision. NM seems to deliver arbitrary results, which are caused by convergence problems. The runtime comparison in Table 10 shows that BFGS is always the fastest algorithm, followed by NLM which is as fast as in the first simulation setting. The runtimes of CG, VaZh and HoCr increased by a factor 2-4 compared to Table 5.
- If more than $n/2$ observations are concentrated in one point, say $\boldsymbol{y}$, the solution of the L_1-median is $\hat{\boldsymbol{\mu}} = \boldsymbol{y}$. A simulation setting as in Section 3.2 but with $n/2 + 1$ observations set to $\boldsymbol{y} = \mathbf{1}$ (vector of ones) has been carried out, expecting the resulting L_1-median estimation to be $\hat{\boldsymbol{\mu}} = \mathbf{1}$. All algorithms are able to find the known center exactly, thus a table showing deviation quantiles can be omitted. However, the computation times differ for some algorithms (Table 11). Although NM converges to the exact solution in this setting, it converges slowly, resulting in a considerably higher value for the runtime. Also NLM is unable to detect this degenerated situation immediately. All other algorithms stop after a single iteration

Distribution	p_{out}	NM	BFGS	CG	NLM	VaZh	HoCr
$N_p(\mathbf{0}, \mathbf{C}))$	0 %	6.42e+03	9.09e-13	0	0	0	0
	10 %	6.01e+03	3.64e-12	0	0	0	0
	20 %	5.66e+03	1.82e-13	0	0	0	0
	30 %	5.36e+03	7.28e-12	0	0	0	0
	40 %	5.27e+03	7.28e-12	7.28e-12	7.28e-12	0	7.28e-12
$LN_p(\mathbf{0}, \mathbf{C})$	0 %	1.08e+04	1.82e-12	9.09e-14	9.09e-14	0	1.82e-12
	10 %	1.08e+04	3.82e-12	0	0	0	0
	20 %	1.12e+04	7.28e-12	0	0	0	0
	30 %	1.23e+04	1.46e-11	0	0	0	0
	40 %	1.40e+04	0	0	0	0	0

Table 9 95% error quantiles of L_1-median estimations applied to collinear data.

Distribution	p_{out}	NM	BFGS	CG	NLM	VaZh	HoCr
$N_p(\mathbf{0}, \mathbf{C})$	0 %	0.266	0.047	0.094	0.078	0.258	0.446
	10 %	0.266	0.047	0.125	0.078	0.250	0.422
	20 %	0.266	0.047	0.195	0.078	0.250	0.406
	30 %	0.265	0.047	0.172	0.078	0.250	0.391
	40 %	0.266	0.047	0.125	0.078	0.282	0.422
$LN_p(\mathbf{0}, \mathbf{C})$	0 %	0.266	0.047	0.109	0.093	0.235	0.422
	10 %	0.266	0.054	0.148	0.093	0.266	0.453
	20 %	0.266	0.047	0.133	0.093	0.250	0.382
	30 %	0.266	0.047	0.125	0.079	0.328	0.469
	40 %	0.265	0.039	0.125	0.094	0.406	0.578

Table 10 Median runtimes [seconds] of the L_1-median algorithms applied to collinear data.

and thus converge so quickly, that the used method for measuring time is not able to record such short periods.

The algorithms HoCr and VaZh have to be pointed out here, as they can handle such occurrences separately: both algorithms are based on the distances of each observation to the current L_1-median estimation, which is calculated during each iteration. By simply checking how many observations have zero distance to the current L_1-median estimation, the method can detect such cases and stop the iteration. A different return code is provided in order to inform the user about such rare occurrences.

Distribution	p_{out}	NM	BFGS	CG	NLM	VaZh	HoCr
$N_p(\mathbf{0}, \mathbf{C})$	0 %	0.265	0.000	0.000	0.047	0.000	0.000
	10 %	0.266	0.000	0.000	0.047	0.000	0.000
	20 %	0.266	0.000	0.000	0.047	0.000	0.000
	30 %	0.266	0.000	0.000	0.047	0.000	0.000
	40 %	0.266	0.000	0.000	0.047	0.000	0.000
$LN_p(\mathbf{0}, \mathbf{C})$	0 %	0.266	0.000	0.000	0.047	0.008	0.000
	10 %	0.265	0.000	0.000	0.047	0.000	0.000
	20 %	0.265	0.000	0.000	0.047	0.000	0.000
	30 %	0.266	0.000	0.000	0.047	0.000	0.000
	40 %	0.266	0.000	0.000	0.047	0.000	0.000

Table 11 Median runtimes [seconds] of the L_1-median algorithms applied to the degenerated data structure.

Although the here examined situations would rarely occur, it is important to keep in mind that there might be further data configurations which are not so easy to handle.

3.6 Real data examples

For testing the L_1-median algorithms on real data, the data sets `bhorizon`, `chorizon`, `humus`, `moss`, `bssbot` and `bsstop`, from the R-library `mvoutlier` are used. These data contain the concentration of chemical elements in the soil of certain regions of Europe. Depending on the considered data set, 600 to 800 observations are available for 30-110 variables. Overall, the data are usually right-skewed, and therefore the algorithms were additionally run on the log-transformed data. Moreover, there are many equal values (especially for `bsstop`) which are caused by detection limit problems (see Reimann et al, 2008). Table 12 gives the deviations as returned by the different algorithms. Since the tolerance levels have been adjusted before, all methods perform similar, again with the exception NM. A comparison of runtimes in Table 13 shows that NLM is constantly the fastest approach, outperforming all other algorithms in terms of computation time, while maintaining the highest accuracy.

Data set	log	NM	BFGS	CG	NLM	VaZh	HoCr
`bhorizon`	no	1.46e+03	0	0	0	0	0
	yes	1.73	0	0	0	0	0
`chorizon`	no	4.99e+04	0	0	0	0	0
	yes	95.3	0	0	0	0	0
`humus`	no	501	0	0	0	2.33e-10	0
	yes	1	4.55e-13	0	0	0	0
`moss`	no	317	0	0	0	0	0
	yes	0.225	2.27e-13	0	0	0	0
`bssbot`	no	80.5	0	0	0	0	0
	yes	32.1	4.55e-13	0	0	0	0
`bsstop`	no	71.5	0	0	0	0	0
	yes	35.5	0	0	0	0	0

Table 12 Deviations of L_1-median algorithms applied to real data sets.

4 Conclusions

For computing the L_1-median, several specific algorithms can be found in the literature. In addition, the solution can also be found by general optimization routines, which are widely available in modern software packages. A fair comparison of these approaches is only possible by a unified software implementation. This has been done in the R-library `pcaPP` (version 1.8-1), using C++ code for the implementation. The implemented algorithms have been tested for various data configurations. Optimization based on NLM leads to the smallest value of the target function in all considered settings, which makes it the first choice as an appropriate algorithm for computing the L_1-median. Moreover, the computation time of this approach turned out to be to a large extent unaffected by the used distribution family, the outlier proportion added, the convergence criterion, and even by high correlation values, whereas other

Data set	log	NM	BFGS	CG	NLM	VaZh	HoCr
`bhorizon`	no	0.047	0.000	0.062	0.016	0.063	0.046
	yes	0.047	0.031	0.125	0.016	0.016	0.016
`chorizon`	no	0.172	0.062	0.219	0.047	0.094	0.156
	yes	0.156	0.078	0.063	0.031	0.063	0.078
`humus`	no	0.031	0.016	0.016	0.000	0.047	0.046
	yes	0.046	0.016	0.094	0.016	0.031	0.016
`moss`	no	0.031	0.000	0.016	0.000	0.031	0.031
	yes	0.031	0.015	0.016	0.000	0.032	0.031
`bssbot`	no	0.109	0.016	0.047	0.016	0.078	0.094
	yes	0.109	0.031	0.031	0.016	0.031	0.047
`bsstop`	no	0.094	0.015	0.047	0.016	0.063	0.047
	yes	0.094	0.062	0.328	0.015	0.047	0.032

Table 13 Runtimes [seconds] of the L_1-median algorithms applied to real data sets.

algorithms tend to have convergence issues in some simulation settings. In the tested situations NLM never showed any problems with convergence, and hence it provides a stable, fast and reliable approach, returning results with the highest precision among the tested algorithms.

Considering the tested data sets and their dimensions, it might be surprising that the absolute runtime of the algorithms is very low. Thus, whenever a robust data center needs to be computed, the L_1-median is an attractive estimator as long as affine equivariance is not required. It is definitely more attractive than the component-wise median, which has the same breakdown point, but which is not orthogonal equivariant.

Concluding, we recommend the algorithm NLM, implemented as `l1median_NLM` in the R-library `pcaPP` (version 1.8-1), as this particular approach turned out to deliver results of highest precision in combination with very low computation time, widely unaffected by the underlying data structure.

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